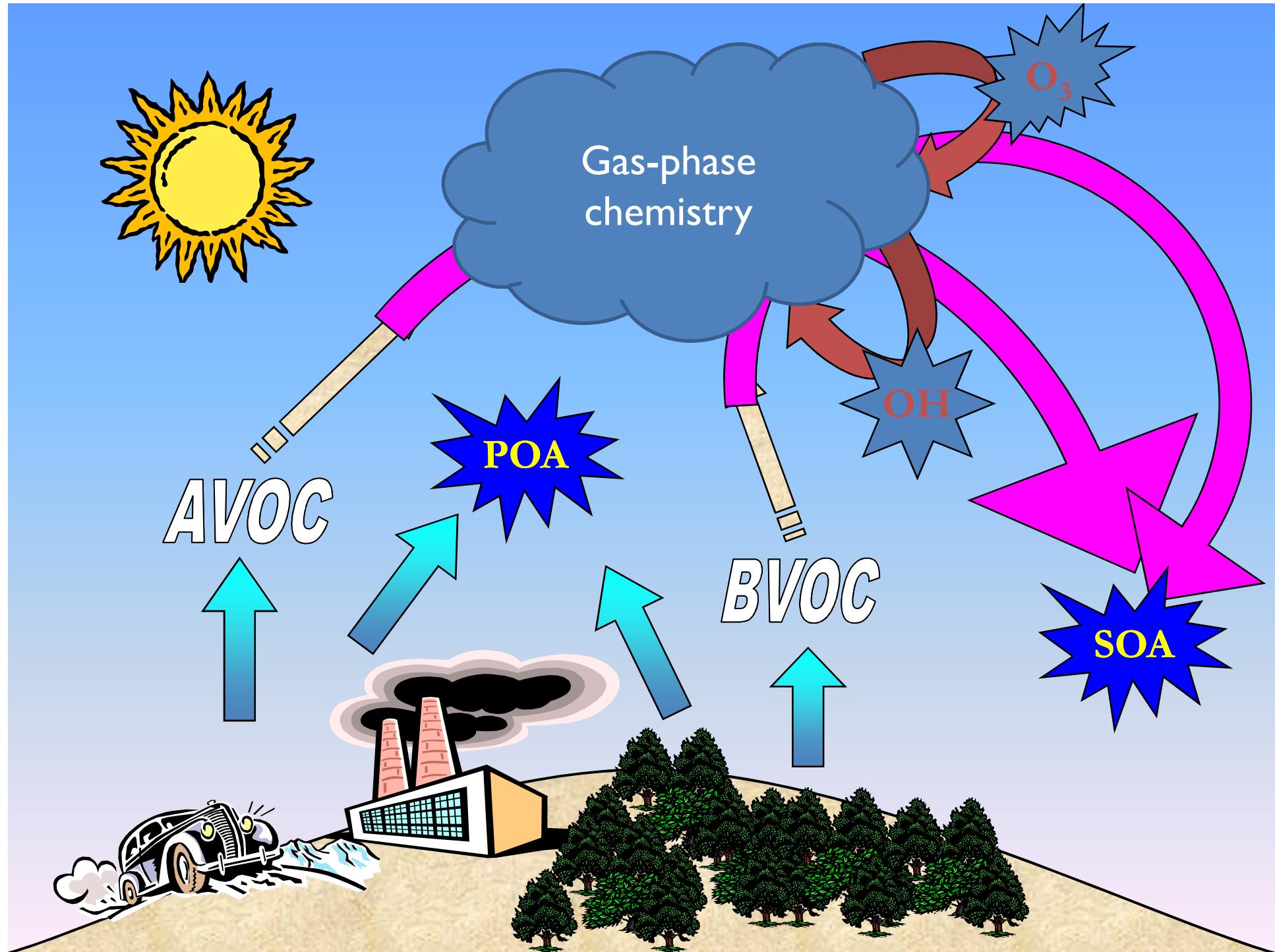




# Secondary organic aerosol representation in global models

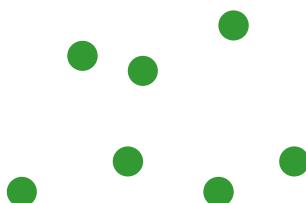
Kostas Tsigaridis (NASA/GISS)

Stelios Myriokefalitakis, Maria Kanakidou (ECPL,UoC)



# SOA production

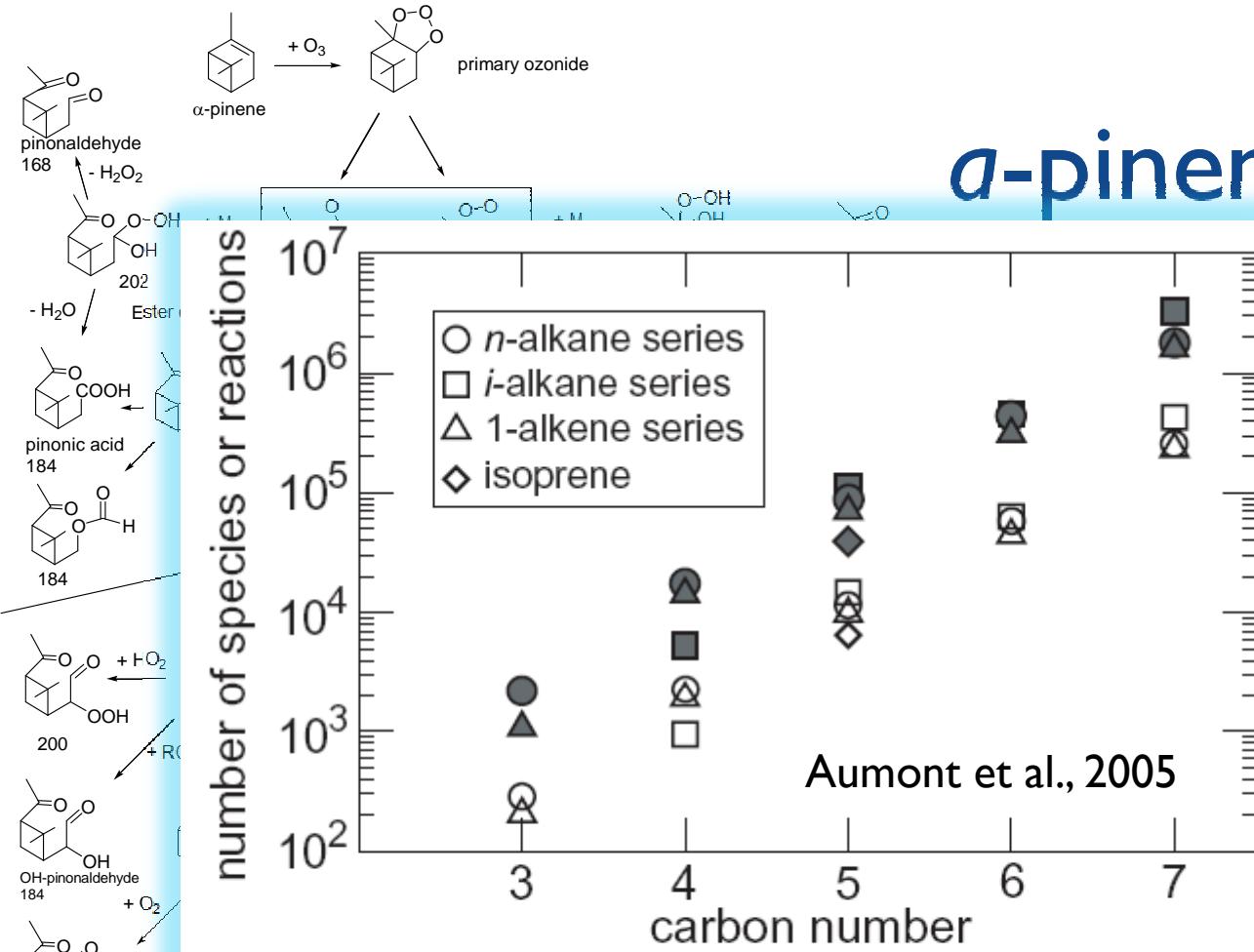
gas-phase  
condensable products



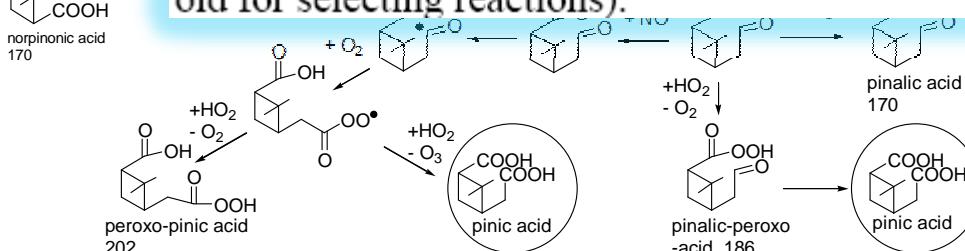
$$G_i = \frac{A_i}{K_{p,i} M_o}$$

absorbing  
aerosol phase

Potential of total evaporation → ~~Upper limit of SOA formation~~ of SOA formation



**Fig. 5.** Number of species (open symbols) and reactions (grey symbols) created by the generator for various series (using a 5% threshold for selecting reactions).

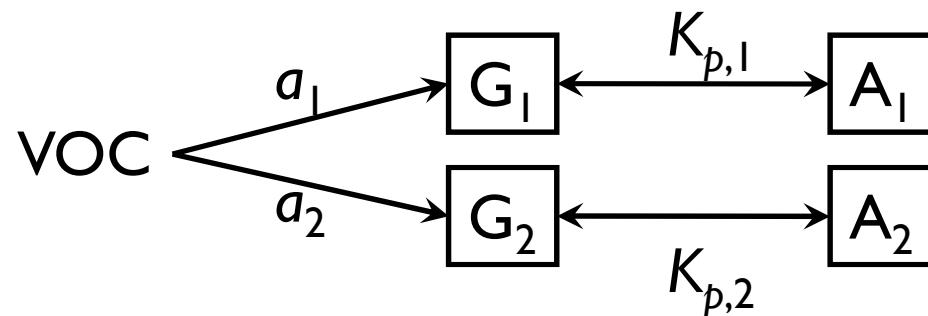




# VOC candidates

- BVOC
  - Isoprene (C5)
  - Monoterpenes (C10, isoprene x 2)
  - Sesquiterpenes (C15, isoprene x 3)
  - higher terpenoid compounds (C>15)
  - others?
  
- AVOC
  - Aromatics (C $\geq$ 6)
  - Solvents (C $\geq$ 4)
  - high C-chain hydrocarbons (C>)
  - others?

# SOA formation – 2 product model



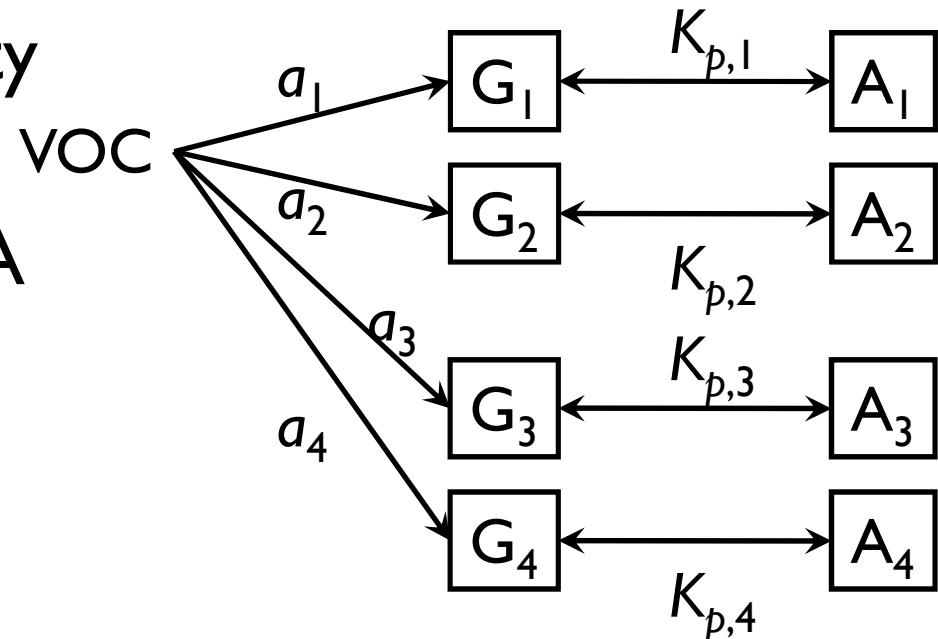
- Keep critical information on:
  - Chemical speciation
  - Optical properties
  - Hydrophilic/hydrophobic behaviour

$$G_i = \frac{A_i}{K_{p,i} M_o}$$

# Processes affecting SOA production

- Pre-existing aerosols
- Oxidant levels
- Temperature
- Gas-phase chemical composition (high/low NO<sub>x</sub>)
- Relative humidity
- UV light
- Evaporated POA
- Aged SOA
- Others?

$$G_i = \frac{A_i}{K_{p,i} M_o}$$

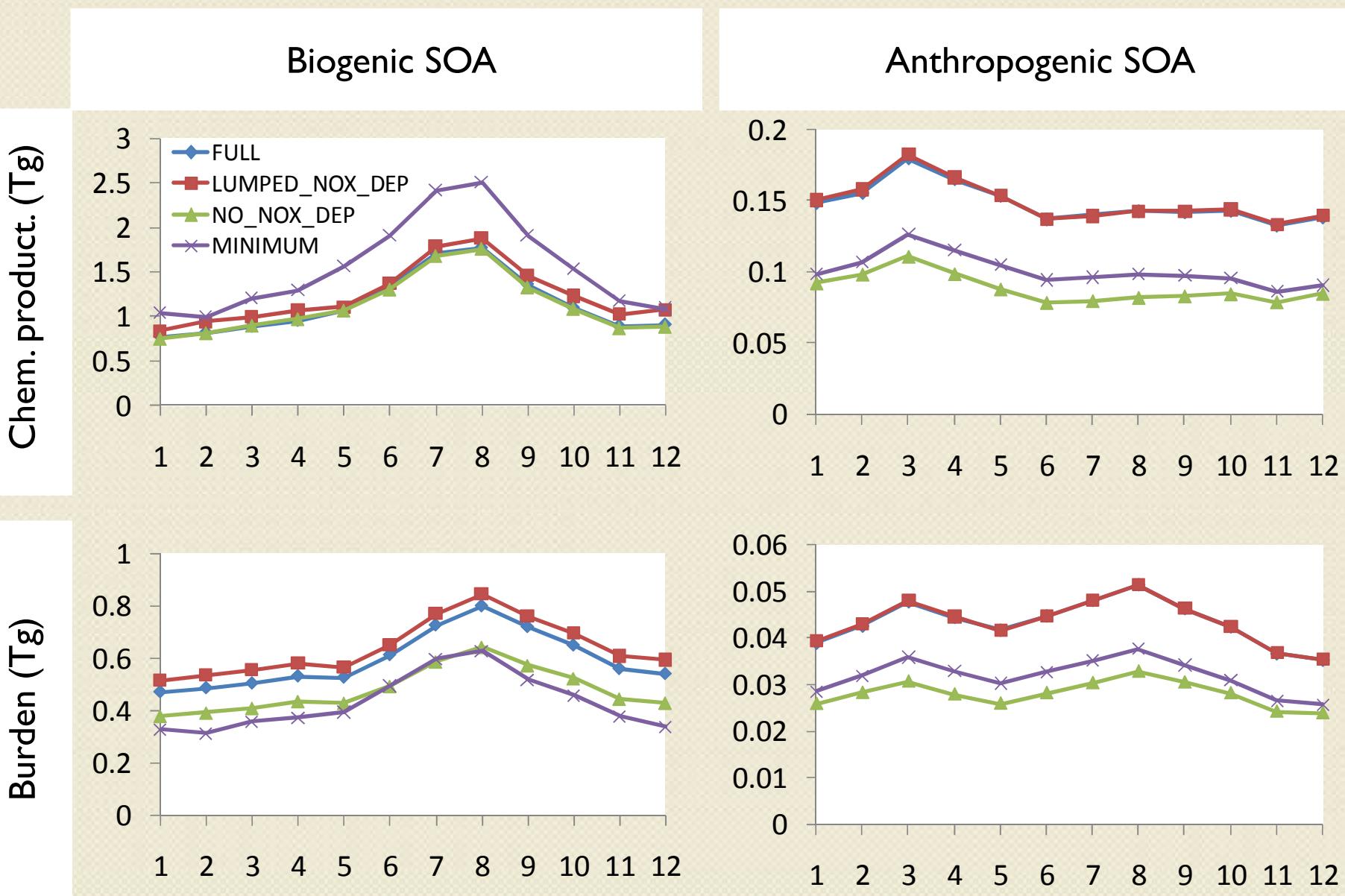




# The simulations – TM3 model

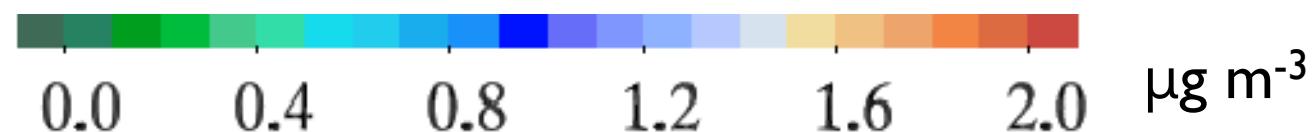
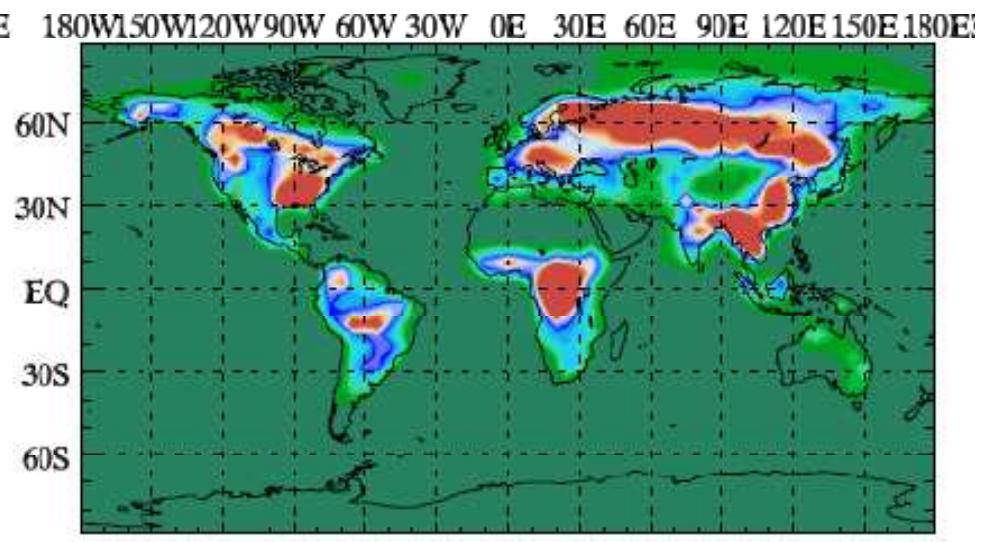
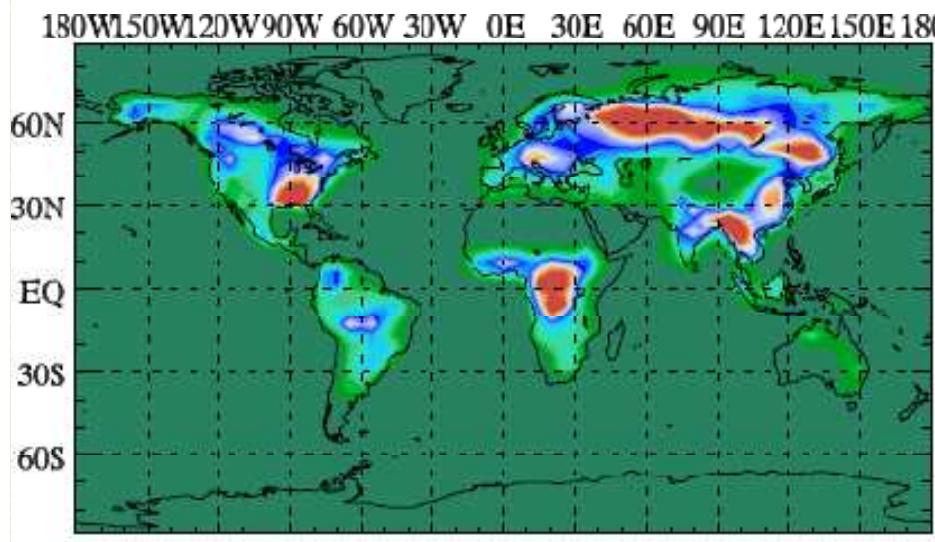
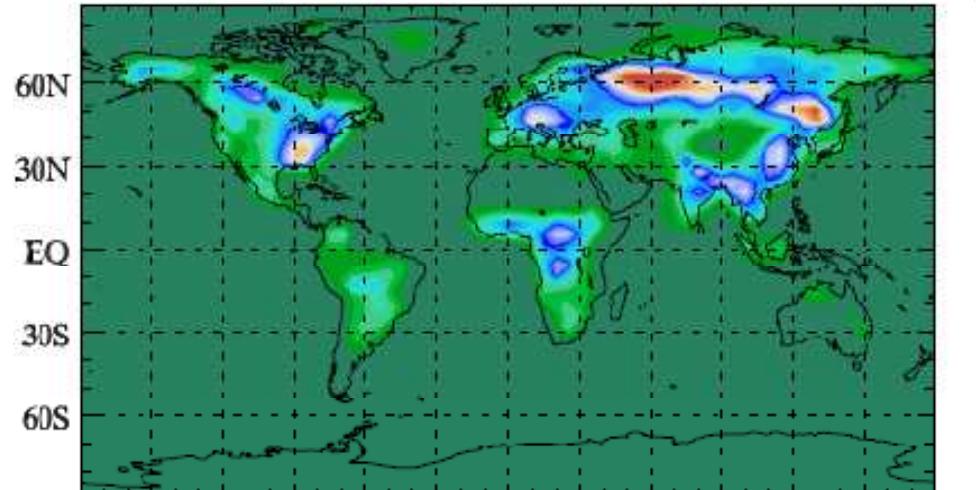
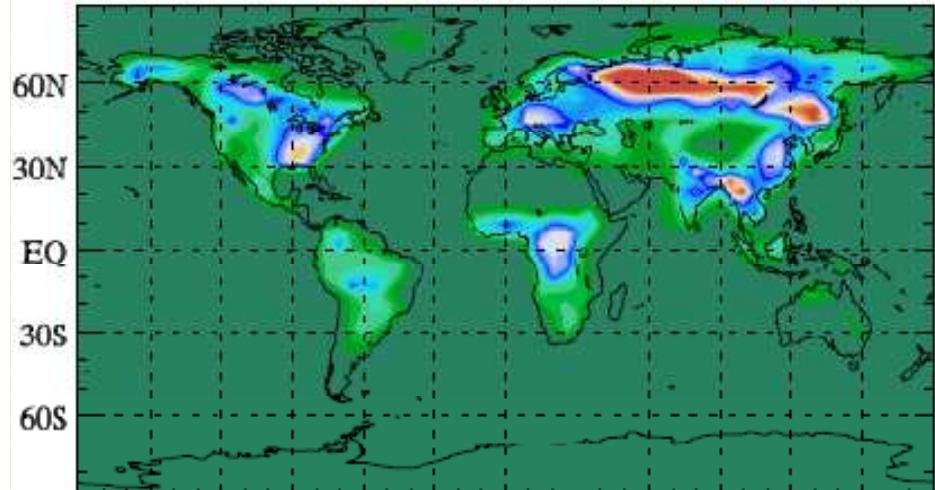
- **FULL (25 SOA-related species)** (Tsigaridis and Kanakidou, AE, 2007)
  - 5 precursors (isoprene,  $\alpha$ -pinene,  $\beta$ -pinene, toluene, xylene)
  - 4 products per precursor (2 high- $\text{NO}_x$ , 2 low- $\text{NO}_x$ )
- **LUMPED\_NOX\_DEP (15 SOA-related species)**
  - 5 precursors (isoprene,  $\alpha$ -pinene,  $\beta$ -pinene, toluene, xylene)
  - 2 products per precursor (high- $\text{NO}_x$  or low- $\text{NO}_x$ , depending)
- **NO\_NOX\_DEP (15 SOA-related species)**
  - 5 precursors (isoprene,  $\alpha$ -pinene,  $\beta$ -pinene, toluene, xylene)
  - 2 products per precursor (low- $\text{NO}_x$ )
- **MINIMUM (9 SOA-related species)**
  - 3 precursors (isoprene,  $\alpha$ -pinene, toluene)
  - 2 products per precursor (low- $\text{NO}_x$ )

# SOA budget

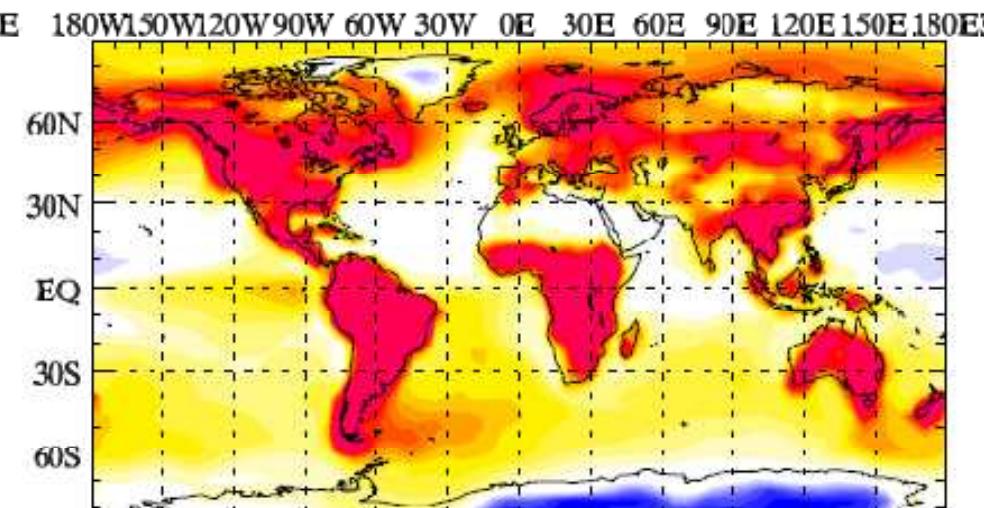
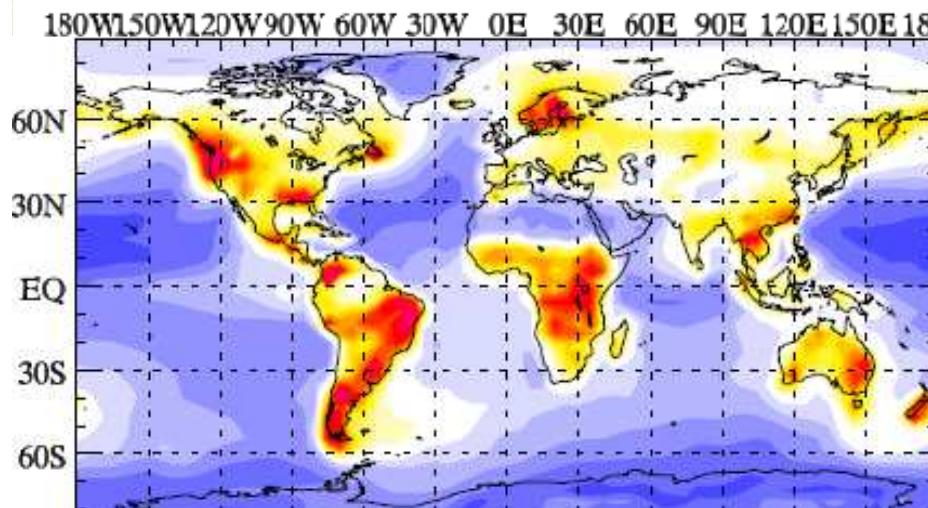
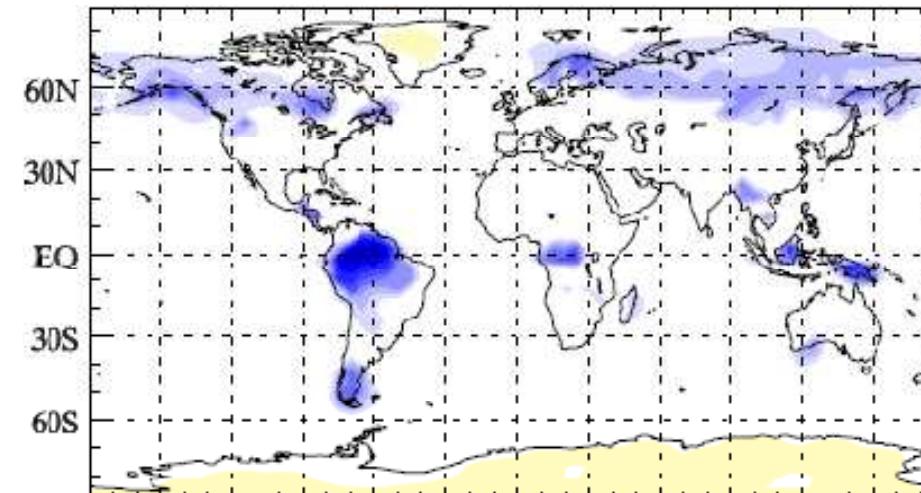
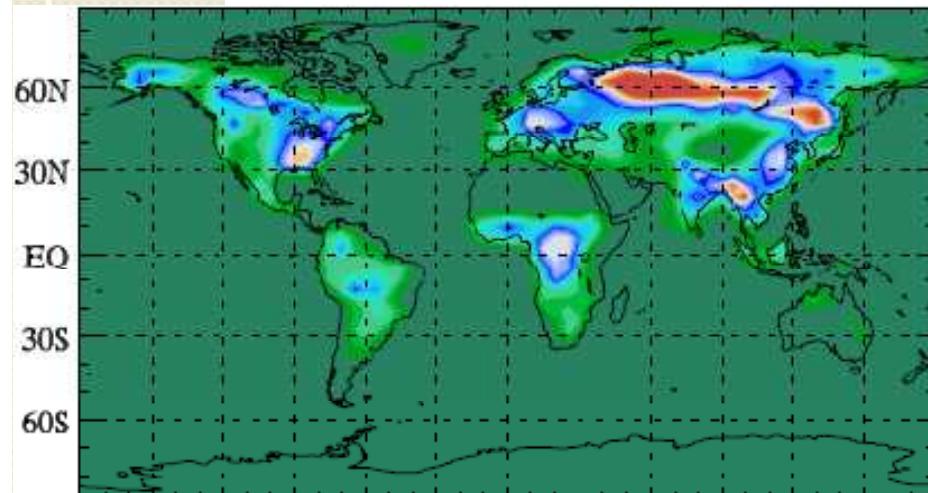


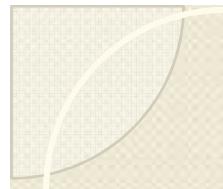


# SOA surface, annual mean

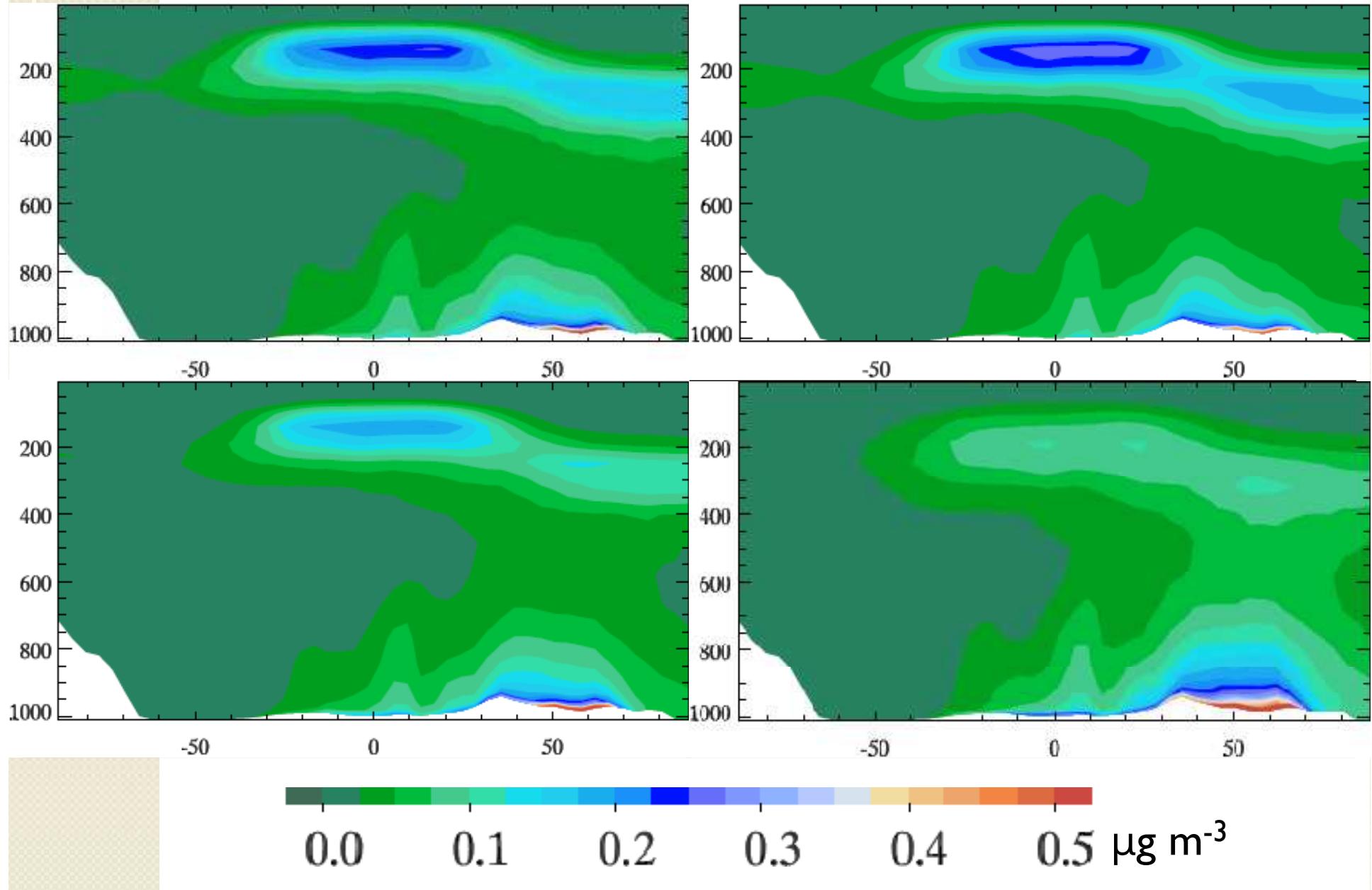


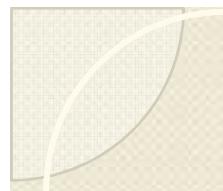
# % difference – surface



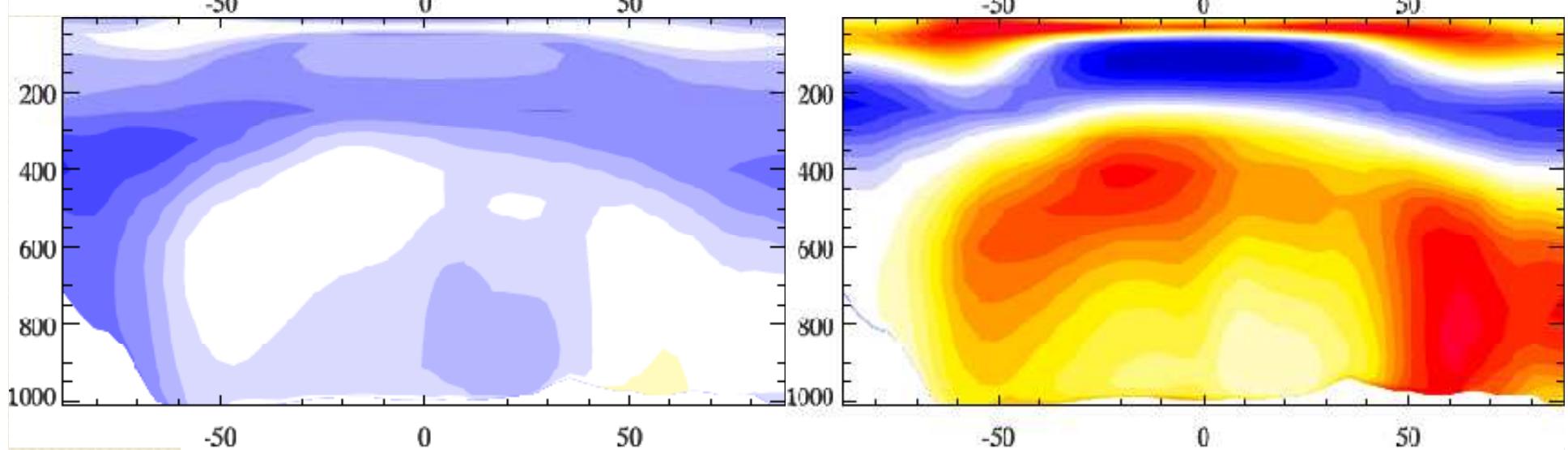
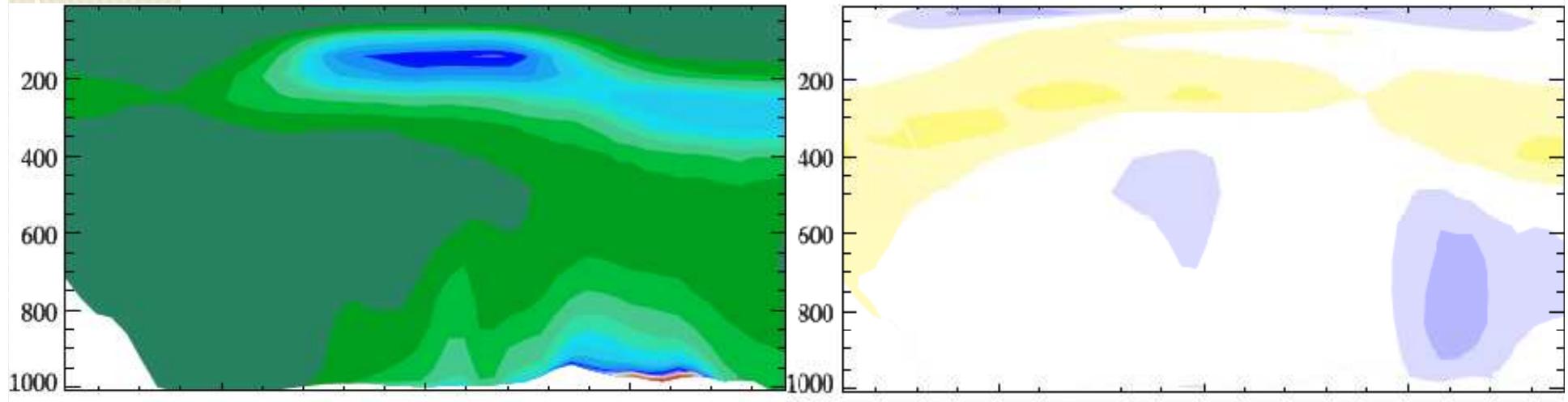


# SOA zonal mean, annual mean

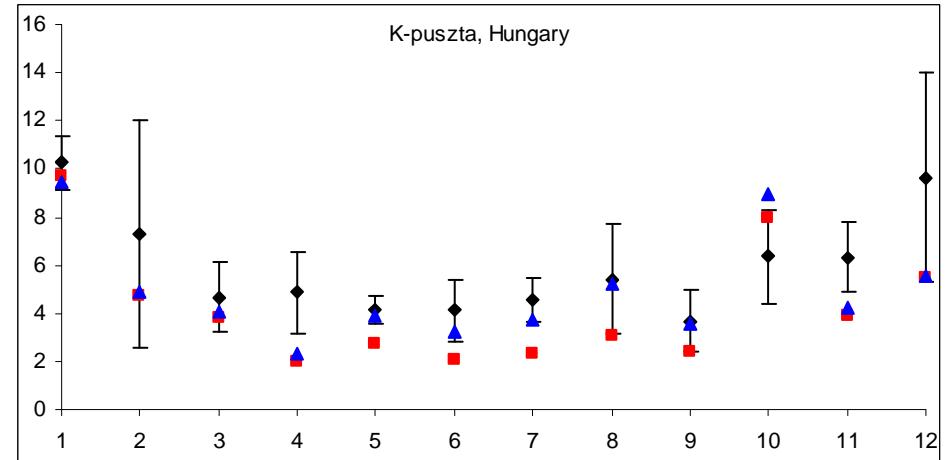
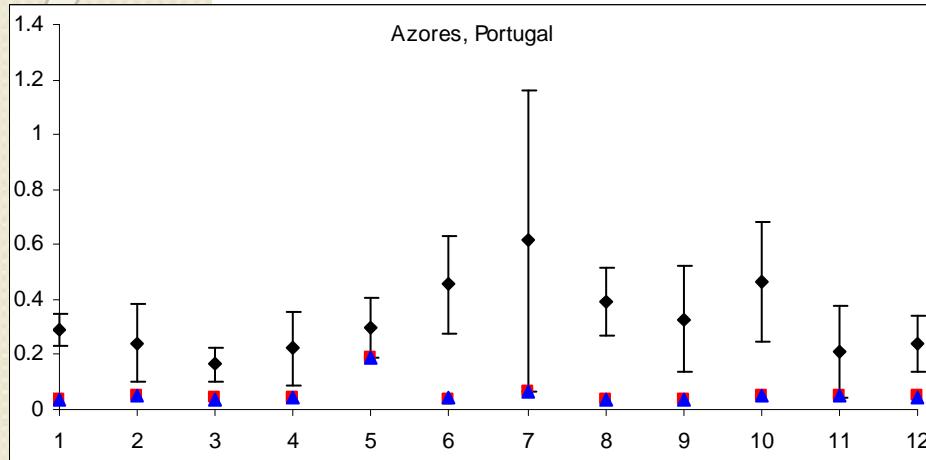




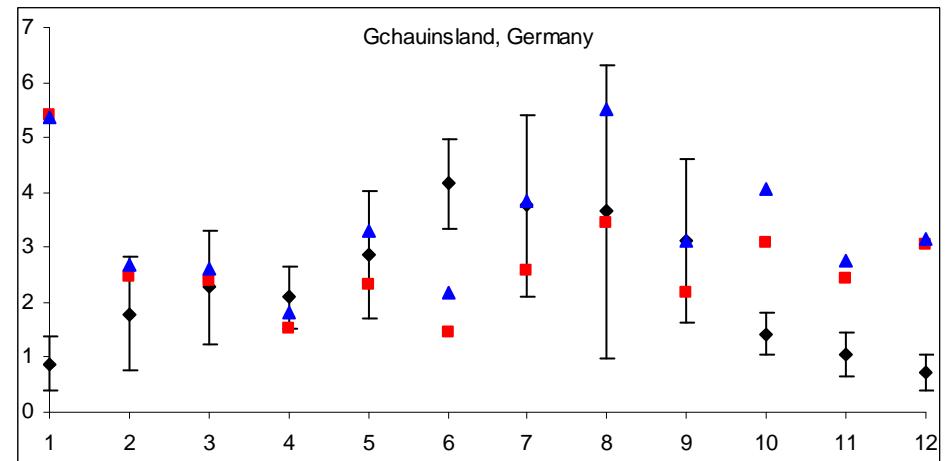
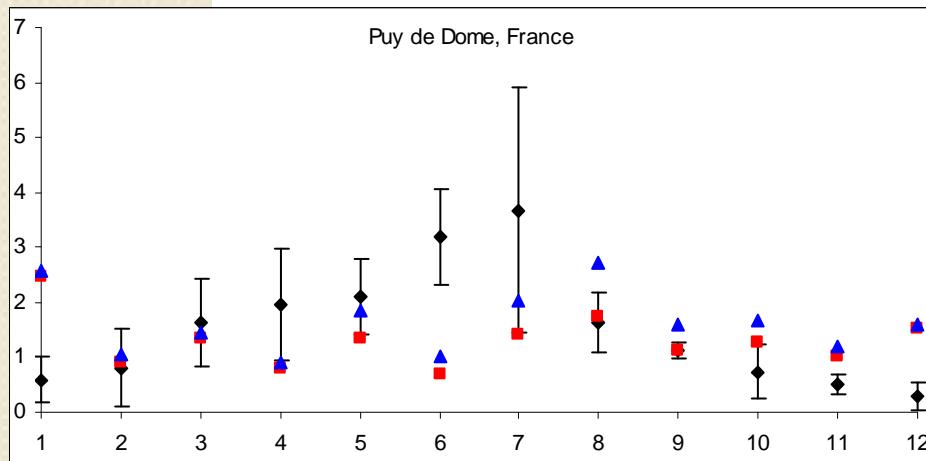
# % difference – zonal mean



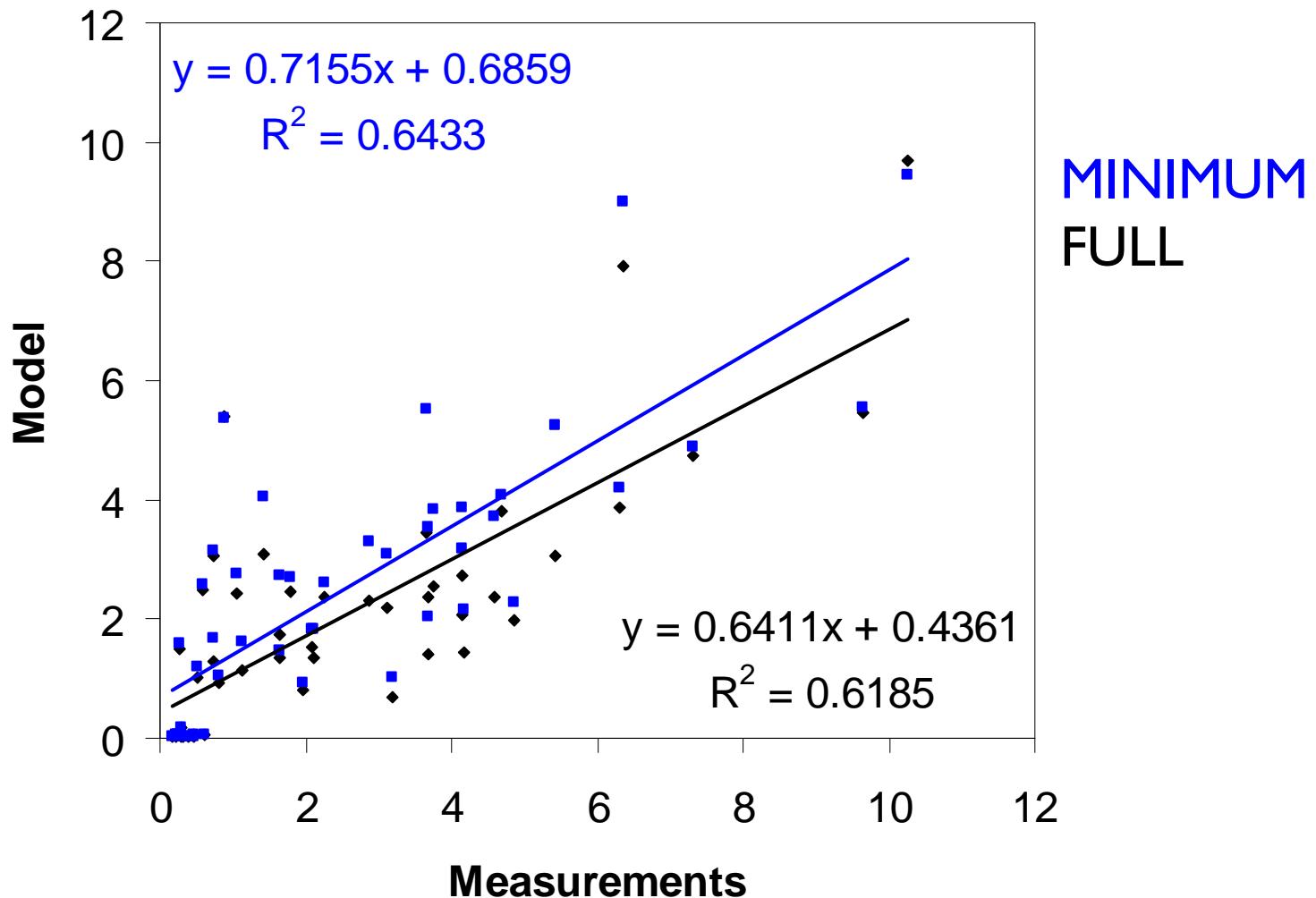
# Comparison with measurements: CARBOSOL



Measurements  
**MINIMUM**  
**FULL**



# Comparison with measurements: CARBOSOL



Units are  $\mu\text{gC m}^{-3}$ , OM/OC = 1.3



# Conclusions and perspectives

- Burden differences compared to surface concentration changes reveal the importance of the free tropospheric SOA.
- Distinction between POA and SOA is important in understanding why models and measurements (dis)agree. Emissions play a major role. This, though, might never happen (POA is semi-volatile; Donahue et al., 2006; Robinson et al., 2007).
- How should we treat the VOC mixture reactivity?
- Update the SOA formation mechanism by including the most recent chamber data of  $\Delta H$ ,  $a$  and  $K_p$  (Offenberg et al., 2006; Henze et al., 2007; Svendby et al., 2008). How should we treat sesquiterpenes ( $\text{NO}_x$  dependence)?
- Detailed comparison with measurements around the globe, ideally not only at surface.
- Thorough study of all different simulations.



# Seminar announcements

- **Maria Kanakidou** (ECPL, professor at the department of chemistry, university of Crete and president of CACGP):  
**August 1, 11 a.m, 3<sup>rd</sup> floor.**
- **Kostas Tsigaridis** (NASA/GISS): Columbia Friday seminar series,  
**September 26, 11 a.m, 3<sup>rd</sup> floor.**